HL 37: Nitrides II – Designed properties and LED

Time: Thursday 9:30–11:00 Location: POT/0006

HL 37.1 Thu 9:30 POT/0006

Designing Visible-Spectrum Nitride Alloys from First Principles — •Jan M. Waack[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany

Precise band-gap engineering across the full visible spectrum is essential for emerging applications such as integrated RGB LEDs. This tunability can be achieved through alloying narrow-band-gap materials like InN or ScN with wide-band-gap semiconductors such as GaN or AlN. Among these systems, random alloys including (In,Ga)N and (Al,Sc)N require advanced theoretical treatments–such as the coherent potential approximation (CPA) and special quasi-random structures (SQS)–to capture their configurational disorder accurately.

In this work, we combine first-principles density functional theory with efficient electronic-structure methods such as LDA-1/2 and the mBJ functional to provide a comprehensive dataset for both random and ordered alloy phases. We report key structural properties including lattice parameters and bond lengths as well as elastic constants, phonon modes, thermodynamic stability, and electronic characteristics such as band gaps and Bloch spectral functions. These results offer a robust theoretical foundation for experimental detection of ordering phenomena and for the rational design of nitride alloys with tailored optical and electronic properties.

HL 37.2 Thu 9:45 POT/0006

Detailed nano-characterization of structural and optical properties of a red-emitting InGaN LED — •N. Dreyer[1], F. Bertram[1], G. Schmidt[1], J. Christen[1], Z. Chen[2], and X. Wang[2] — [1]Otto-von-Guericke-University Magdeburg, Germany — [2]Peking University, Beijing, China

A fully processed and operating red InGaN LED was grown by MOVPE on a GaN/sapphire template. The active region, which consists of three identical stacks, is surrounded by n- and p-GaN with an EBL. Each stack contains three quantum wells with different indium concentrations: two with a low indium concentration for strain relaxation, and one subsequently grown red-emitting quantum well (RQW). The structure was characterized using scanning transmission electron microscopy (STEM) and the orientation of the Burgers vector (edge- or screw type dislocation) was determined. Cross-sectional cathodoluminescence performed directly in STEM shows broad band-to-band recombination in the n-GaN at $T = 17$ K which is caused by band gap renormalization and conduction band filling. Line shape analysis of this emission band yields a charge carrier density of 6×10^{18} cm^{-3}. The vertical evolution of the RQW emission exhibits a shift of 123 meV within the active region. Furthermore, the lateral homogeneity of the RQW emission will be examined. A blue-shift of the RQW emission of up to 365 meV was found around defects. The vertical and lateral trapping processes of excess carriers will be discussed in detail. The capture length of the bottom RQW was found to be 78 nm using highly spatially resolved vertical linescans across the active region.

HL 37.3 Thu 10:00 POT/0006

Determination of optical losses in AlGaN-based multi-mode waveguides — •Verena Kowallik[1], Martin Guttmann[2], Leonardo Wildenburg[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute for Physics & Astronomy, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

Many applications for ultraviolet photonic integrated circuits (UV PICs), such as biochemical sensing, atomic clocks, and UV Raman spectroscopy, require materials with a large bandgap energy to facilitate low optical losses. One possible candidate are AlGaN alloys which are already successfully employed for the fabrication of UV light emitting diodes (UV-LEDs) and UV lasers. However, the optical properties of AlGaN materials, especially the absorption losses have not yet been studied in detail in the UVC spectral range. In this work, the absorption losses in 200 μm wide n-$Al_{0.76}Ga_{0.24}N$ waveguides were investigated using monolithically integrated UV-LEDs emitting at 262 nm and detectors. By Monte Carlo ray-tracing simulations, we identified different contributions of the optical losses, namely, the propagation losses and scattering losses. Here, we implemented the waveguide surface roughness determined from atomic force microscopy images. Also, we investigated the portion of rays reaching the detector without beeing guided in the waveguide, e.g. scattered at the substrate's backside or the AlN/sapphire interface.

HL 37.4 Thu 10:15 POT/0006

Influence of the AlGaN multi-quantum well design on the efficiency of 233 nm far-UVC LEDs grown by MOVPE — •Rebekah Seonggyeong Kim[1], Marcel Schilling[1], Massimo Grigoletto[1,2], Jakob Höpfner[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Physics and Astronomy, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

Light emitting diodes (LEDs) emitting in the far ultraviolet-C (far-UVC) spectral range are promising for applications like skin safe disinfection and gas sensing. The composition and thickness of the AlGaN-multi quantum wells and barriers are crucial for the efficiency of the LEDs. In this work we investigate the impact of the last quantum well barrier's (LB) thickness (0 nm to 10 nm) and aluminum mole fraction (76% - 86%) onto the electrooptical performance of the LEDs. The LEDs with an aluminum mole fraction of 80 % and a thickness of 5 nm exhibit the highest external quantum efficiency (EQE) of 0.32 % at 16 mA (on-wafer).

HL 37.5 Thu 10:30 POT/0006

In-rich InGaN quantum well growth for green InGaN LED — •Christoph Berger, Armin Dadgar, and André Strittmatter — Otto-von-Guericke-University, Magdeburg, Germany

Achieving high-efficiency green InGaN LEDs remains challenging due to material issues like phase instability, metallic inclusions and interface roughening. We present an optimized MOVPE growth approach that significantly improves the optical and morphological quality of green LEDs. After each QW, a growth interruption combined with a controlled temperature ramp is introduced before starting the GaN barrier growth. This sequence allows to get rid of excess indium that accumulates on the surface during QW growth, leading to smoother interfaces, a removal of indium-rich defects visible in Nomarski microscopy and consequently, a substantial suppression of a grayish appearance of the wafer. We further combine this process with hybrid MQW designs, where blue QWs are grown below a green top QW, leading to an improvement of the efficiency of the LED. The impact of different growth sequences and layer designs on the optical and structural characteristics of green LEDs will be discussed.

HL 37.6 Thu 10:45 POT/0006

Nano-characterization of polarization-doped deep UV LED structures using highly spatially resolved cathodoluminescence spectroscopy — •E. Bäker[1], F. Bertram[1], G. Schmidt[1], N. Dreyer[1], J. Christen[1], T. Kolbe[2], S. Hagedorn[2], H.K. Cho[2], J. Rass[2], S. Einfeldt[2], and M. Weyers[2] — [1]Otto-von-Guericke-University Magdeburg, Germany — [2]Ferdinand-Braun-Institut (FBH), Germany

AlGaN-based deep UV LEDs emitting below 250 nm are of great interest for many applications. Especially in the far-UVC, efficient p-doping poses major challenges, which can be effectively overcome by the concept of polarization doping. This study compares far-UVC LEDs with different AlGaN composition gradients used for polarization doping. The LEDs were grown by MOVPE on optimized AlN/sapphire templates. While the n-side of the diode uses conventional Si-doping, the p-side utilizes an AlGaN-layer with constant [Ga]-gradient. Diodes with different [Ga]-gradients but identical thicknesses are analyzed, with the Ga mole fraction increasing linearly from 0.02 to 0.45 and from 0.02 to 0.81, respectively. Using low temperature cathodoluminescence spectroscopy directly performed in a scanning transmission electron microscope, a nano-scale correlation of the optical properties with the real structure is obtained. Cross-sectional CL line scans show the different emission of the gradient layer. While the sample with the shallow gradient shows continuous emission spectral red-shift from 240 nm to 260 nm, the sample with the steep gradient shows an abrupt jump from 273 nm to 312 nm, indicating lattice relaxation.